

Methanol
67-56-1 | DTXSID2021731

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.54

Global applicability domain: Inside

Local applicability domain index: 4.99e-01

Confidence level: 7.24e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N,N-Dimethylformamide</div> <div>Measured: 7.94e-01</div> <div>Predicted: 1.12</div>	<div>Image not found</div> <div>Thiourea</div> <div>Measured: 2.00</div> <div>Predicted: 2.11</div>	<div>Image not found</div> <div>Dimethyl sulfoxide</div> <div>Measured: 3.98</div> <div>Predicted: 4.07</div>
<div>Image not found</div> <div>1,4-Dioxane</div> <div>Measured: 5.01e-01</div> <div>Predicted: 1.06</div>	<div>Image not found</div> <div>Morpholine</div> <div>Measured: 2.82</div> <div>Predicted: 1.87</div>	